Table 1 Energies are relative to the lowest energy structure for each composition. Note that the final structure after geometry optimisation may have a very different symmetry from the starting structure.

Starting structure	Final space group	Lattice parameters	No. of atoms per unit cell	Energy (DFT) / (eV atom^{-1})	Comment
SiN					
β-InS	$Pmnn$	a=2.85 Å, b=4.73 Å, c=7.15 Å	8	0	cif file available
GaSe	$P\bar{1}$	a=2.86 Å, b=2.87 Å, c=6.88 Å, α=86.5°, β=84.2°, γ=60.1°	4	0.18	Symmetry reduced during optimisation; cif file available
Rocksalt	$Fm\bar{3}m$	a=4.20 Å	8	1.47	
GeN					
β-InS	$Pmnn$	a=3.03 Å, b=4.89 Å, c=7.46 Å	8	0	cif file available
GaSe	$P\bar{1}$	a=3.01 Å, b=3.01 Å, c=7.32 Å, α=91.6°, β=94.3°, γ=119.3°	4	0.14	Symmetry reduced during optimisation; cif file available
Rocksalt	$Fm\bar{3}m$	a=4.36 Å	8	0.81	
SiP					
β-InS	$Pmnn$	a=3.67 Å, b=4.45 Å, c=8.75 Å	8	0	cif file available
GaSe	$P\bar{1}$	a=6.01 Å, b=3.56 Å, c=7.94 Å, α=92.6°, β=90.0°, γ=90.0°	8	0.01	Symmetry reduced during optimisation; cif file available
Zincblende	$Cmm2$	a=6.93 Å, b=8.05 Å,c=5.20 Å	16	0.27	Symmetry reduced during optimisation
Wurtzite	$Cmcm$	a=4.39 Å, b=6.36 Å, c=4.80 Å	8	0.03	Optimised to the 5-5 structure, cif file available
Rocksalt	$C2/m$	a=7.33 Å, b=6.50 Å, c=4.84 Å β=92.2°	16	0.08	Symmetry reduced during optimisation; cif file available
GeP					
β-InS	$Pmnn$	a=3.78 Å, b=4.47 Å, c=8.90 Å	8	0	cif file availale
GaSe	$P\bar{1}$	a=6.12 Å, b=3.64 Å, c=8.05 Å, α=91.9°, β=90.0°, γ=90.0°	8	0.11	Symmetry reduced during optimisation; cif file available
Zincblende	Cm	a=6.20 Å, b=4.22 Å, c=3.73 Å β=120.2°	4	0.25	Symmetry reduced during optimisation
Wurtzite	$Cmcm$	a=4.53 Å, b=6.50 Å, c=4.94 Å	8	0.06	Optimised to the 5-5 structure, cif file available
Rocksalt	$C2/m$	a=6.16 Å, b=3.38 Å, c=3.74 Å β=125.2°	4	0.05	Symmetry reduced during optimisation; cif file available